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Anisotropic Diffusion in ZPPR Lattices

ELY M. GELBARD

Applied Physics Division Argonne National Laboratory Argonne, Illinois 60439

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Anisotropic Diffusion in ZPPR Lattices

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ABSTRACT

Diffusion coefficients are computed for a typical ZPPR lattice cell using the methods of Benoist and Bonalumi. It is noted that the diffusion coefficients, D, for leakage normal to the plates, as defined by Benoist and by Bonalumi, are both double-valued. The spread between Benoist's x-diffusion coefficients is, in the ZPPR cell, half as large as the difference between D and D. Bonalumi's x-diffusion coefficients are much farther apart, the interval between them being considerably larger than the difference between D and D. Neither the Benoist nor the Bonalumi method yields homogenized diffusion coefficients which preserve fluxes, reaction rates, or eigenvalues. A modified definition of homogenized diffusion coefficients is proposed for one-group problems. The modified parameters are defined so as to quarantee that eigenvalues are preserved in the homogenization process. It is felt that generalization to the multigroup case will not be difficult. The relation between the new diffusion coefficients and the Benoist coefficients is discussed.

I. INTRODUCTION

In published work on the analysis of ZPPR critical experiments $^{\rm l}$ anisotropic diffusion has, so far, been neglected. Such an approach seems reasonable in a first approximation since, at the high energies where most leakage occurs, the ZPPR fuel plates are optically thin. Recent Argonne calculations indicate, however, that in the range from 1-10 MeV, the diffusion coefficients parallel to and perpendicular to the plate surfaces may differ by as much as 4%, and that in some ZPPR assemblies this difference will induce an 0.8% change in $k_{\rm eff}^{\rm \ 2}$. Thus, while anisotropic diffusion effects in ZPPR criticals are normally not very large, neither are they negligible.

A great many methods are available for the treatment of anisotropic diffusion in heterogeneous assemblies. It is not our intention here, however, to survey all these methods or to elaborate the intricate relations between them. Instead we focus our attention on only two, namely, Benoist's method 3 and the more recently developed method of Bonalumi. 4

Benoist's method is well-known and has been widely used, apparently with great success. Nevertheless important questions about the accuracy and range of validity of this method remain, and seem to require further attention. One finds, for example, that there is in the literature no detailed analysis of the accuracy of the Benoist method in slab cells like those of the ZPPR lattice. It may be argued that, if Benoist's method is adequate for the treatment of thermal reactor lattices, it must surely be adequate in ZPPR lattices where the fuel is relatively thin and heterogeneity effects are relatively small. But, precisely because the fuel plates are thin, the flux in and near the plates is highly anisotropic 5

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whereas Benoist's method is based on the approximation that it is isotropic. It seems proper, then, to question the validity of this as well
as other Benoist approximations before relying on the Benoist method for
the analysis of ZPPR critical assemblies.

A more fundamental question is raised by Bonalumi, 4 who objects to Benoist's definition of effective diffusion coefficients, and proposes another. Benoist's and Bonalumi's methods do not differ radically from each other, and they share with other methods some seemingly universal features. Apparently all methods discussed in the literature on anisotropic diffusion assume, first, that in the lattice an overall buckling, \underline{B} , is superimposed on a periodic flux; secondly, that the leakage associated with this buckling can be expanded in a Taylor series in the components of \underline{B} ; and, finally, that the buckling is small enough so that only leading terms in such a series need be retained. But the methods of Benoist and Bonalumi, despite these similarities, yield diffusion coefficients which, in a typical ZPPR lattice, are substantially different from each other. Clearly, then, one is called upon to establish a rationale for choosing between these methods before either is used for the analysis of ZPPR critical assemblies.

It should be noted that *both* the Benoist and Bonalumi definitions give us double-valued diffusion coefficients, though this point seems to have been overlooked in the literature. We shall see that the spread between the permissable values of D normal to the plates is rather large if we accept Bonalumi's definition. If instead, we accept Benoist's definition, this spread becomes considerably smaller.

Both the Bonalumi and Benoist definitions of D seem somewhat arbitrary. We shall show that, in a nonmultiplying medium, neither yields whereas demoter's method is based on the approximation that, is taked the terms of the salvest devotes. It evens propert than, to exception the walldisty of this salvest terms as the salvest period for the entry salvest the entry salvest of the entry salvest period for the entry salvest of the entry salvest the entry salvest of the entry salvest of the entry salvest of the entry salvest the entry salvest of the entry salvest

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fluxes and absorption rates which match those in the original heterogeneous lattice, and neither gives the right eigenvalue when fission is present. Thus, there seems to be room for still another definition and, in closing, we propose a definition which, in one energy group, *does* give the right eigenvalue. It seems likely that this definition can be reformulated easily for multi-energy problems, though this has not yet been done.

II. THE METHODS OF BENOIST AND BONALUMI IN SLAB LATTICES

We begin by deriving Benoist's and Bonalumi's equations specialized to slab lattices. Of course, derivations for general geometries already exist in the literature. It is our purpose, in rederiving these equations, to develop our notation and to exhibit all implied approximations as clearly as possible.

$$\hat{\Omega} \cdot \nabla F(\underline{r}, \hat{\Omega}) + \Sigma_{\underline{t}} F(\underline{r}, \hat{\Omega}) = (1/4\pi) \Sigma_{\underline{s}} (\underline{r}) \phi(\underline{r}) + (1/4\pi) S(\underline{r}) . \tag{1}$$

We assume that, in the slab lattice, ⁶

$$S(\underline{r}) = q(x) \cos (\underline{B} \cdot \underline{r}) = R\{q(x) e^{i\underline{B} \cdot \underline{r}}\},$$
 (2)

where q(x) has the periodicity of the lattice. Correspondingly,

$$F(\underline{r},\hat{\Omega}) = R\{f(x,\hat{\Omega}) e^{i\underline{B}\cdot\underline{r}}\}, \qquad (3)$$

and

$$\phi(\underline{r}) = R\{\chi(x) e^{i\underline{B}\cdot\underline{r}}\}, \qquad (4)$$

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where, again, f and χ have the periodicity of the lattice. Note that f and χ are generally complex. Inserting Eqs. (2), (3), and (4) into Eq. (1), we find that

$$\hat{\Omega} \cdot \nabla f(x, \hat{\Omega}) + \left[\Sigma_{t}(x) + i(\hat{\Omega} \cdot \underline{B})\right] f(x, \hat{\Omega}) = (1/4\pi)\Sigma_{s}\chi(x) + (1/4\pi)q(x) . (5)$$

Let

$$R(x,\hat{\Omega}) = R\{f(x,\hat{\Omega})\}, \quad I(x,\hat{\Omega}) = I\{f(x,\hat{\Omega})\}, \quad (6)$$

$$\rho(x) = R\{\chi(x)\}, \qquad \psi(x) = I\{\chi(x)\}.$$
 (7)

Then, from Eqs. (5) and (6),

$$\hat{\Omega} \cdot \nabla R(x, \hat{\Omega}) + \Sigma_{t} R(x, \hat{\Omega}) = (1/4\pi) \Sigma_{s}(x) \rho(x) + (1/4\pi) q(x) + (\hat{\Omega} \cdot \underline{B}) I(x, \hat{\Omega}), \qquad (8)$$

$$\hat{\Omega} \cdot \nabla I(x, \hat{\Omega}) + \Sigma_{t} I(x, \hat{\Omega}) = (1/4\pi) \Sigma_{s}(x) \psi(x) - (\hat{\Omega} \cdot \underline{B}) R(x, \hat{\Omega}) . \qquad (9)$$

Now we expand R and I in Taylor series in the two variables B_x and B_y :

$$R(x,\hat{\Omega}) = \sum_{n,m=0}^{\infty} B_{x}^{n} B_{y}^{m} R^{(n,m)}(x,\hat{\Omega}), \qquad (10)$$

$$I(x,\hat{\Omega}) = \sum_{n,m=0}^{\infty} B_{x}^{n} B_{y}^{m} I^{(n,m)}(x,\hat{\Omega}) . \tag{11}$$

It can easily be shown that $I^{(0,0)} = 0$, and that the leading terms in Eqs. (10) and (11) satisfy the equations:

$$\mu \frac{\partial R^{(0,0)}}{\partial x} + \Sigma_t R^{(0,0)} = \frac{\Sigma_s}{4\pi} \int d\hat{\Omega} R^{(0,0)} + \frac{1}{4\pi} q(x) , \qquad (12)$$

t can easily be shown that ((0,0) = 0, and that upe leading cases in

$$\mu \frac{\partial I^{(0,1)}}{\partial x} + \Sigma_t I^{(0,1)} = \frac{\Sigma_s}{4\pi} \int d\hat{\Omega} I^{(0,1)} - \Omega_y R^{(0,0)}, \text{ (see Ref. 7)}$$
 (13)

$$\mu \frac{\partial I^{(1,0)}}{\partial x} + \Sigma_t I^{(1,0)} = \frac{\Sigma_s}{4\pi} \int d\hat{\Omega} I^{(1,0)} - \mu R^{(0,0)}, \qquad (14)$$

where

$$\mu \equiv \Omega_{\mathbf{x}}$$
.

From Eqs. (3), (6), and (7) we see that, to first order in B,

$$F(\underline{r},\hat{\Omega}) = R^{(0,0)} \cos (\underline{B} \cdot \underline{r}) - I_1 \sin (\underline{B} \cdot \underline{r}), \qquad (15)$$

$$I_1 \equiv B_x I^{(1,0)} + B_y I^{(0,1)}$$
 (16)

The current, \underline{J} , is, by definition, given by the expression

$$\underline{J} = \int \hat{\Omega} d\hat{\Omega} \left[R^{(0,0)} \cos (\underline{B} \cdot \underline{r}) - I_1 \sin (\underline{B} \cdot \underline{r}) \right]$$

$$= J_0 \cos (\underline{B} \cdot \underline{r}) + J_1 \sin (\underline{B} \cdot \underline{r}) , \qquad (17)$$

where

$$\underline{J}_0 \quad \equiv \quad \int \hat{\Omega} \ d\hat{\Omega} \ R^{(0,0)} \ , \qquad \underline{J}_1 \quad \equiv \quad - \int \hat{\Omega} \ d\hat{\Omega} \ I_1 \ .$$

Let \mathbf{x}_{L} and \mathbf{x}_{R} be, respectively, the left- and right-hand cell boundaries. Since we are dealing with a lattice consisting of infinite slabs, we may define the upper and lower horizontal boundaries arbitrarily. In any case the net leakage, L, out of the cell is given by the expression

$$L = \int_{cell} \nabla \cdot \underline{J} \, dv . \tag{18}$$

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From Eqs. (3), (6), and (7) we see that, to start order of 5,

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Now we note, first, that $R^{(0,0)}$ satisfies reflecting boundary conditions at x_L and x_R . Secondly (since $R^{(0,0)}$ is the flux in the cell when $\underline{B}=0$), it is clear that \underline{J}_0 lies in the x direction, i.e., $\underline{J}_0=\underline{J}_{0x}$. Therefore,

$$\int_{\text{cell}} \nabla \cdot \left[\underline{J}_0 \cos \left(\underline{B} \cdot \underline{r} \right) \right] dv = \int_{\text{cell}} (\partial/\partial x) \left[\underline{J}_0 \cos \left(\underline{B} \cdot \underline{r} \right) \right] = 0 . (19)$$

Thus,

$$L = \int_{cell} \nabla \cdot \left[\underline{J}_1 \sin \left(\underline{B} \cdot \underline{r} \right) \right] dV . \qquad (20)$$

Carrying out the differentiation indicated in Eq. (20), we find that

$$L = \int_{cell} \cos (\underline{B} \cdot \underline{r}) \left[\underline{B}_{x} \underline{J}_{1x} + \underline{B}_{x} \underline{J}_{1y} \right] dV + \int_{cell} \sin (\underline{B} \cdot \underline{r}) \nabla \cdot \underline{J}_{1} dV . (21)$$

From Eqs. (13) and (14) we deduce that

$$j_{1,21} = -\int \alpha_x I^{(0,1)} d\hat{\alpha} = 0$$
, (22)

$$j_{1,12} = -\int \Omega_y I^{(1,0)} d\hat{\Omega} = 0$$
 (23)

Therefore,

$$J_{1x} = -B_{x} \int \Omega_{x} I^{(1,0)} d\hat{\Omega} = B_{x} \dot{J}_{1,11}, \qquad (24)$$

$$J_{1y} = -B_{y} \int \Omega_{y} I^{(0,1)} d\hat{\Omega} = B_{y} \dot{J}_{1,22}. \qquad (25)$$

Above, in Eqs. (22)-(25) we have made contact with Benoist's notation: the quantities $j_{1,k'k}$ have precisely the same meaning here as in Benoist's papers. For those not familiar with Benoist's work we point out that the subscript 2 in the symbol $j_{1,21}$ indicates that the current

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Carrying out the differentiation indicated to Eq. (20), we rind coat:

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 $j_{1,21}$ is produced by a source having Ω_y as a factor [see Eq. (13)]. The final subscript, 1, indicates that $j_{1,21}$ is a current in the x direction. Subscripts in the other quantities $j_{1,k}\gamma_k$ have similar meanings.

Since \underline{J}_1 is independent of y

$$\nabla \cdot \underline{J}_1 = B_{\mathbf{x}}(\partial/\partial \mathbf{x})j_{1,11} . \tag{26}$$

Substituting from Eqs. (24), (25), and (26) into Eq. (21), we find that

$$L = \int_{\text{cell}} \cos \left(\underline{B} \cdot \underline{r} \right) \left[\underline{B}_{x}^{2} \underline{j}_{1,11} + \underline{B}_{y}^{2} \underline{j}_{1,22} \right] dV$$

$$+ \underline{B}_{x} \int_{\text{cell}} \sin \left(\underline{B} \cdot \underline{r} \right) (\partial/\partial x) \underline{j}_{1,11} dV . \tag{27}$$

Let \underline{r}_0 be the midpoint of the cell, and assume (as we will in all our future work) that the cell is symmetric. Expanding L in a Taylor series in B_x and B_y, and retaining only leading terms, we find that

$$L = \cos \left(\underline{B} \cdot \underline{r}_{0}\right) \int_{\text{cell}} \left[\underline{B}_{x}^{2} \underline{j}_{1,11} + B_{y}^{2} \underline{j}_{1,22}\right] dV$$

$$+ B_{x} \sin \left(\underline{B} \cdot \underline{r}_{0}\right) \int_{\text{cell}} (\partial/\partial x) \underline{j}_{1,11} dV$$

$$+ B_{x}^{2} \cos \left(\underline{B} \cdot \underline{r}_{0}\right) \int_{\text{cell}} (x - x_{0}) (\partial/\partial x) \underline{j}_{1,11} dV$$

$$+ B_{x} B_{y} \cos \left(\underline{B} \cdot \underline{r}_{0}\right) \int_{\text{cell}} (y - y_{0}) (\partial/\partial x) \underline{j}_{1,11} dV . \tag{28}$$

Since $j_{1,11}$ is independent of y the last term on the right-hand side of Eq. (28) vanishes, and since $j_{1,11}$ is a periodic function of x, the second term also vanishes. Thus,

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$$L = \cos \left(\underline{B} \cdot \underline{r}_{0}\right) \left\{ B_{x}^{2} \left[\int_{cell} j_{1,11} dV + \int_{cell} (x - x_{0})(\partial/\partial x) j_{1,11} dV \right] + B_{y}^{2} \int_{cell} j_{1,22} dV \right\}.$$
(29)

It should be noted that Eq. (29) is an exact expression for the leakage (in the limit B_x , $B_y \rightarrow 0$) if the series in B_x and B_y converges.

At this point Benoist asserts that effective diffusion constants must satisfy the relation

$$L = \left(D_{\mathbf{x}} B_{\mathbf{x}}^2 + D_{\mathbf{y}} B_{\mathbf{y}}^2 \right) \int_{\text{cell}} \phi(\underline{r}) \ dV , \qquad (30)$$

where, as in Eq. (1)

$$\Phi(\underline{r}) = \int F(\underline{r}, \hat{\Omega}) d\hat{\Omega}. \qquad (31)$$

From Eq. (15) it is clear that

$$\phi(\underline{r}) = \cos(\underline{B} \cdot \underline{r}) \int R^{(0,0)} d\hat{\Omega} - \sin(\underline{B} \cdot \underline{r}) \int I_1 d\hat{\Omega} . \qquad (32)$$

But ${\rm I}_1$, as defined in Eq. (16), is first order in B. Therefore, neglecting higher-order terms,

$$\int_{\text{cell}} \Phi(\underline{r}) \ dV = \cos (\underline{B} \cdot \underline{r}_0) \int_{\text{cell}} dV \int_{\mathbb{R}^{(0,0)}} d\hat{\Omega}$$

$$= \cos (\underline{B} \cdot \underline{r}_0) \int_{\text{cell}} \Phi \ dV , \qquad (33)$$

$$\Phi = \int_{\mathbb{R}^{(0,0)}} d\hat{\Omega} \ R^{(0,0)} .$$

It should be noted that (g. (29) is an exact expression for the leakage (for the limit B., B. 0) if the series in B. and B. converges ...

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Thus, to leading terms,

$$L = \left(D_{x}B_{x}^{2} + D_{y}B_{y}^{2}\right) \cos \left(\underline{B} \cdot \underline{r}_{0}\right) \int_{cell} \phi(\underline{r}) dV. \qquad (34)$$

Comparing Eq. (34) with Eq. (29) we conclude that

$$D_{x} = D_{1} = \left[\int_{cell} j_{1,11} dV + \int_{cell} (x - x_{0})(\partial/\partial x) j_{1,11} dV \right] / \int_{cell} \phi dV$$
, (35)

$$D_{y} = D_{2} = \int_{cell} j_{1,22} dV / \int_{cell} \phi dV .$$
 (36)

Given that

$$j_{1,k',k} = 0, k' \neq k$$
 (37)

from Eqs. (22) and (23), and that

$$(\partial/\partial y)j_{1,22} = 0 (38)$$

from Eq. (26), one sees that Eqs. (35) and (36) are precisely, Benoist's equations for D_1 and D_2 specialized to a slab cell.⁹

Certainly it is possible to solve Eqs. (12), (13), and (14) in their present form (by discrete ordinate methods, for example) and to compute diffusion coefficients from Eqs. (35) and (36) directly. In the interests of efficiency, however, Benoist chooses to develop a computational procedure based on specially designed collision probability techniques. To facilitate the use of such techniques he introduces various approximations which we discuss next.

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It is easy to show that $I^{(0,1)}$, defined implicitly via Eq. (13), is proportional to $\Omega_{\mathbf{v}}$, i.e.

$$I^{(0,1)} = \Omega_{y}h(x,\mu), \qquad \mu \frac{\partial h}{\partial x} + \Sigma_{t}h = -R^{(0,0)}, \qquad (39)$$

and it follows that the scattering term in Eq. (13) vanishes. We will assume, in Eqs. (13) and (14), that $R^{(0,0)}$ is almost isotropic, and replace $R^{(0,0)}$ with the scalar flux, ϕ . In this approximation we may write

$$\mu \frac{\partial \hat{h}}{\partial x} + \Sigma_{t} \hat{h} = -\phi , \qquad I^{(0,1)} \approx \hat{I}^{(0,1)} \equiv \Omega_{y} \hat{h} . \qquad (13')$$

Clearly, Eq. (13') can be solved without difficulty through the use of collision probabilities.

Now suppose that we set out to solve Eq. (14), as well, by collision probability methods, with $R^{(0,0)}$ replaced by ϕ . We see that the "uncollided flux," $I_{unc}^{(1,0)}$, produced by the source $\mu\phi$, is given by the expression

$$I_{unc}^{(1,0)} = \mu \hat{h}$$
,

where, again,

$$\mu \frac{\partial \hat{\mathbf{h}}}{\partial \mathbf{x}} + \Sigma_{\mathbf{t}} \hat{\mathbf{h}} = -\phi .$$

If we assume that \hat{h} is isotropic, as is usual in collision probability calculations, then $I_{unc}^{(1,0)}$ is proportional to μ and the scattering integral again vanishes. Thus, the uncollided flux is the whole flux and we may write

$$\mu \frac{\partial \hat{h}}{x} + \Sigma_{t} \hat{h} = -\phi$$
, $I^{(0,1)} \gtrsim \hat{I}^{(0,1)} \equiv \mu \hat{h}$. (14')

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Clearly, Eq. ([5]) can be solved without difficulty through the use of golfischen probenijters.

probability methods, with $R^{(0,0)}$ replaced by 4. We see that the "uncollisted flux," $I^{(2,0)}$ produced by the source as: is given by the expression.

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It turns out that, if the scattering is <u>not</u> isotropic, and $\bar{\mu}$ is the mean cosine of the scattering angle, then

$$\mu \frac{\partial \hat{h}}{\partial x} + \Sigma_{t} \hat{h} = \frac{\bar{\mu} \Sigma_{t}}{4\pi} \int \hat{h} d\hat{\Omega} - \phi , \qquad I^{(1,0)} \approx \hat{I}^{(1,0)} \equiv \mu \hat{h} ;$$

but anisotropic scattering is a nonessential complication here and we shall continue to assume that the scattering is isotropic.

The numerator on the right-hand side of Eq. (35) contains two terms: the first is the volume integral of $\mathbf{j}_{1,11}$, a quantity readily computed by collision probability methods. The computation of the second term is somewhat more difficult. One finds, however, that the second term is often small and the neglect of this term is generally considered to be part of what is called "Benoist's Method". In brief, then, Benoist's approximate diffusion constants are given by Eqs. (35') and (36'),

$$\hat{D}_{1} = \int_{cell} \hat{j}_{1,11} dV / \int_{cell} \phi dV , \qquad \hat{j}_{1,11} = - \int \Omega_{x} \hat{I}^{(1,0)} d\hat{\Omega} , (35')$$

$$\hat{D}_{2} = \int_{cell} \hat{j}_{1,22} dV / \int_{cell} \phi dV , \qquad \hat{j}_{1,22} = - \int \Omega_{y} \hat{I}^{(0,1)} d\hat{\Omega} , (36')$$

with $\hat{I}^{(1,0)}$ and $\hat{I}^{(0,1)}$ determined by Eqs. (13') and (14'), respectively.

On retracing the arguments that lead from Eq. (18) to Eq. (35), it will be seen that, to leading terms in the components of \underline{B} ,

$$D_{x} = D_{1} = \int_{cell} (\partial/\partial x) (J_{x}) dV / B_{x}^{2} \int_{cell} \Phi dV . \qquad (40)$$

This expression for D_x follows directly from Eqs. (18) and (30). Undoubtedly Eq. (18) is a valid expression for the net leakage from the cell, but it is not clear how Benoist arrives at Eq. (30). In Benoist's published work

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but anticurrent Scottering is a nonessential complication were and we shall continue to assume that the scattering is isotropic.

The first is the volume incorrate of j_{1,17}, a quantity readily computed by somewhat more difficult. One finds however, that the second term is small and the neglect of this term is generally considered to us part of what is called "Benoist's National". In brief, them, Senoist's Phacaracke diffusion constants are given by Eqs. (35°) and (35°).

with 1^(1,0) and 1^(0,1) determined by Eqs. (13') and (14'), respectively.

On retrocing the arguments that lead from Eq. (18) to Eq. (35), its
will be seen that, to leading texts in the components of 8.

This expression for D, follows directly from Eqs. (18) and (30). Undoubted Eq. (18) is a valid expression for the men leadage from the cell, but it is not clear bow Benoist arrives at Eq. (30). In denoist's published work

the relation is postulated without discussion. It is possible that Benoist considers that Eq. (30) is intuitively obvious: but, on the other hand, Bonalumi rejects this relation completely. Instead Bonalumi takes, as his definition of D_{φ} , the expression

$$D_{\mathbf{x}}(\mathsf{BON}) = \int_{y_{\mathbf{L}}}^{y_{\mathbf{U}}} J_{\mathbf{x}}(x_{\mathbf{R}}, y) \, dy \left\{ B_{\mathbf{x}} \frac{\int_{y_{\mathbf{L}}}^{y_{\mathbf{U}}} \left[\Phi(x_{\mathbf{R}}, y) - \Phi(x_{\mathbf{L}}, y) \right] \, dy}{T} \right\}, \tag{41}$$

$$T = x_{\mathbf{R}} - x_{\mathbf{L}}.$$

Here $\mathbf{y}_{\mathbf{U}}$ and $\mathbf{y}_{\mathbf{L}}$ are, respectively, the y coordinates of the upper and lower cell boundaries. It is easy to show that in slab geometry the right-hand side of Eq. (41) will be independent of the values chosen for these coordinates. After trivial manipulation we find that

$$D_{x}(BON) = j_{1,11}(x_{B}) / \phi(x_{B})$$
, (42)

where x_B is the x coordinate of either cell boundary. In Eq. (42) we have used the notation $D_x(BON)$ to make a sharp distinction between Bonalumi's D_x and the diffusion coefficients derived from Benoist's postulate, Eq. (30).

As was apparently first pointed out by Bonalumi, 4 Eq. (35), the equation defining Benoist's "exact" diffusion coefficient D_1 , can be cast into a form quite similar to that of Eq. (42). After integrating over y in Eq. (35), then integrating by parts over x, we find that

$$D_{1} = j_{1,11}(x_{B}) / \overline{\phi}_{cell} ,$$

$$\overline{\phi}_{cell} = \int_{x_{L}}^{x_{R}} \phi(x) dx / T .$$
(43)

the relation is postulated without discursion. It is possible that benefits possible that benefit that the (20) is insultively covious but, on the other benefit booking related this relation vampletely. Instead monitors of D. the expression

Here y and y are respectively, the y coordinates of the upper and lower cell boundaries. It is easy to shretcat in slap geometry the right-hand shae of En. (41) will be independent of the values closen for these coordinates. After trivial manipulation on that

where x, is the x coordinate of either cell boundary. To in iq. (42) we have used the noistion D (40) so make a sharp distinction Detween Bonalumi's by and the diffusion coefficients Cerived from Bendick's postulate. Eq. (20). As was apparently first cointed out by Bonalumi's Eq. (35), the equa-

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It will be seen that Eqs. (42) and (43) are identical except that in Eq. (42) the denominator is the cell-edge flux while in Eq. (43) it is the average flux. For this reason Bonalumi refers to his diffusion constant as "cell-edge normalized".

Perhaps it is fair to say that both Eqs. (40) and (41) seem perfectly plausible as definitions of the x diffusion coefficient. In arguing for the use of Eq. (41) in place of Eq. (40), Bonalumi asserts that the celledge normalized $D_{\rm x}$ (BON) satisfies Selengut's equivalence relation while Benoist's D_1 does not, but this assertion is stated without proof. The relation between Benoist's and Bonalumi's x diffusion coefficient will be discussed further in later sections.

III. DOUBLE VALUE OF D_x

In Eqs. (42) and (43) various fluxes and currents are evaluated at the cell boundary. But in a symmetric cell there are two different sets of symmetry planes and correspondingly, two sets of cell boundaries (see Fig. 1). Thus there are two possible values of D_1 , and of D_{x} (BON). It is easy to show that this ambiguity in the x diffusion coefficient is not simply due to a weakness in the definition but is inherent, in a sense, in the underlying physics. Suppose that $\Sigma(x)$ is the cross section for some arbitrarily chosen reaction in the lattice. Then the average reaction rate, $\overline{A}(x_0,B^2)$, within the cell is given by the expression

$$\bar{A}(x_0, B^2) = \int_{x_L}^{x_R} dx \ \Sigma(x) \int d\hat{\Omega} \ F(x, \hat{\Omega}) / T , \qquad (45)$$

$$\bar{A}(x_0, B^2) = (1/T) \int_{x_L}^{x_R} dx \ \Sigma(x) \left[\cos \left(B_x x \right) R(x, \hat{\Omega}) - \sin \left(B_x x \right) I(x, \hat{\Omega}) \right] d\hat{\Omega} \ . (46)$$

(AZ) the denominator is the cell-edge fire smile in Eq. (43) at its that in Eq. (43) at its the denominator is the cell-edge fire smile in Eq. (43) at its the decrease flux. For this reason bonelum refers to mis diffusion constant as "cell-edge normalized".

Perhaps It is fair to say that both Eqs. (4D) and (41) and perfectly plausible as definitions of the a distriction coefficient. In arguing for the use of Eq. (41) in place of Eq. (40), Donajumi asserts that the cell-edge normalized D_g (80%) suctafies Selection is acateal enter relation while Benoist's D₁ does not, but this assertion is stated without proof. The relation between Benoist's and Bonalum's x diffusion coefficient will be discussed further in later sections

III. DOUBLE WALDE, OF B.

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Here we have arbitrarily set \mathbf{y}_0 = 0; note that $\bar{\mathbf{A}}(\mathbf{x}_0,\mathbf{B}^2)$ is a function of \mathbf{x}_0 in the sense that it is the average reaction rate in a cell whose center is at \mathbf{x}_0 . Equation (46) is obtained by substituting from Eqs. (3) and (4) into Eq. (45). Now assume, for the sake of simplicity, that $\mathbf{B}_{\mathbf{y}}$ = 0. One can then show from Eqs. (8) and (9) that $\psi(\mathbf{x}) \equiv \int d\hat{\Omega} \ \mathbf{I}(\mathbf{x},\mu)$ is antisymmetric in \mathbf{x} about \mathbf{x}_0 . It follows that, to order \mathbf{B}^2 ,

$$\bar{A}(x_0, B^2) = \frac{\cos (B x_0)}{T} \left\{ \int_{x_L}^{x_R} dx \ \Sigma(x) \rho(x) - \frac{1}{2} B^2 \int_{x_L}^{x_R} dx \ (x - x_0)^2 \Sigma(x) \psi(x) - B \int_{x_L}^{x_R} dx \ (x - x_0) \Sigma(x) \rho(x) \right\}.$$
(47)

Note that, since $\psi(\textbf{x})$ is of order B, the last term in brackets is actually of order $B^2,$ so that we may write

$$\bar{A}(x_0, B^2) = \frac{\cos (B x_0)}{T} \left[\int_{x_L}^{x_R} dx \ \Sigma(x) \rho(x) - c B^2 \right]. \tag{48}$$

Here, of course,

$$\rho(x) \equiv \int d\hat{\Omega} R(x,\mu) , \qquad \psi(x) \equiv \int d\hat{\Omega} I(x,\mu) , \qquad (49)$$

and

$$c = \frac{1}{2} \int_{\mathbf{x}_{T}}^{\mathbf{x}_{R}} dx (x - x_{0})^{2} \Sigma(x) \rho(x) + \int_{\mathbf{x}_{T}}^{\mathbf{x}_{R}} dx (x - x_{0}) \Sigma(x) \psi(x) . \quad (50)$$

ore we have appreciately set y_0 a y_0 in note that $f(x_0, \mathbb{R}^n)$ is a function of y_0 in the sense that its the average reaction rate in a cell whose center f(x) at x_0 , education (45) to obtained by substituting from Eqs. (1) and (4) at f(x) is a function show even Eqs. (8) and (9) that g(x) is a transpositive in about y_0 . It follows that, to order g(x).

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Note that, since v(x) is of order the last term in erackers is actually of order B. so that we may write

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Since Σ and ρ have the periodicity of the lattice, the integral in Eq. (48) is uniquely defined. On the other hand, it is clear from Eq. (50) that c can have either of two possible values, one for each of the two possible definitions of the unit cell.

Thus, the reaction rate (regarded as a function of x_0) has a cosine distribution over the lattice but there are two possible values one can assign to the amplitude of the cosine. Accordingly there will be two sets of "equivalent" homogenized cross sections which give reaction rates that match the cell-averaged reaction rates in the lattice. If the reaction rates and fluxes in the equivalent homogenized medium are to be correct at $B^2 = 0$, and if the effective cross sections are to be independent of buckling, then we must take

$$\overline{\Sigma} = \int_{x_L}^{x_R} \Sigma(x) \phi(x) dx/T$$
 (51)

to be the homogenized reaction cross section. The two possible values of c then determine two diffusion constants, both equally acceptable.

When, as is customary, we neglect the second term in the numerator Eq. (35), then the diffusion coefficient is uniquely defined by Eq. (35'). It follows that, when such an approximation is valid, the difference between the two possible values of D_1 must be small. If, to the contrary, this second term is not negligible the spread between possible D_1 values may be significant. Usually $\mathbf{j}_{1,11}$ will be positive for all x, and in such cases \hat{D}_1 will lie between these two possible values.

Since E and a nave the pertodicity of the lattice, the integral in Eq. (48) is uniquely defined. On the other hand, it is clear from Eq. (50) that E can have either of two possible values, one for each of the Ext possible definitions of the unit cell.

Thus, the reaction rate (regarded as a function of xo) has a coalnu distribution over the lattice but there are two possible values one can assign to the emplitude of the cosine. Accordingly there will be two sets of "equivalent" nonequalized cross sections which give reaction rates that match the cell-everaged reaction rates in the lattice. If the reaction rates and fluxes in the equivalent homogenized medium are to be compact at Br = 0, and if the effective cross sections are to be independent of buckling, then we must take

(13)
$$T(x) \phi(x) \phi(x) 2^{\frac{x^2}{2}} = \frac{x}{2}$$

to be the homogenized reaction cross section. The two possible values of c. then determine two diffusion constants, both equally acceptable.

Mhen, as is customary, we neglect the second term in the numerator Eq. (35), then the diffusion coefficient is uniquely dufland by Eq. (35'). It follows that, when such an approximation is valid, the difference bear the two possible values of 0, must be small. If, to the contrary, this vacond turn is not negligible the spread between possible 0, values may be significant. Usually 1, 1, 1 will be possible for all 8, and in such cases 0, will its between possible values.

IV. NUMERICAL RESULTS

We propose, in this section: (1) to investigate the accuracy, in a typical ZPPR lattice, of the various approximations which are usually considered to be part of "Benoist's Method"; (2) to examine the differences in numerical values of $D_{\mathbf{x}}$ computed via cell-edge and cell-averaged normalization; and finally, to determine how large an uncertainty is introduced into $D_{\mathbf{x}}$ by the ambiguity in the definition of cell boundaries.

A. Diffusion Parallel to Plates

It turns out that cell-edge and cell-average normalization give the same expression for D_y , so that there is, in this case, no difference between the definitions proposed by Benoist and Bonalumi. Both lead us to Eq. (36). After carrying out the y integration in Eq. (36) we get

$$D_{y} = \int_{x_{L}}^{x_{R}} j_{1,22} dx / \int_{x_{L}}^{x_{R}} \phi dx . \qquad (52)$$

Since D_y depends solely on integrals over the cell, and not on point values, it makes no difference which of the two alternative sets of symmetry planes we choose as cell boundaries: both choices give the same D_y . On the other hand, there is, of course, a difference between D_y and D_y .

In a series of numerical experiments we have used the ANISN code 12 to compute the functions h and \hat{h} . This can be done, of course, in many ways, but we find it convenient to adopt the following procedure:

(1) We treat Eqs. (12) and (39) as the Group 1 and Group 2 equations, respectively, of a two-group set, with $\Sigma_{s\ell}^{1\to2} = -(2\ell+1)/2$. Here $\Sigma_{s\ell}^{1\to2}$ is the ℓ 'th Legendre component of the scattering cross section from Group 1 into Group 2.

We propose in this sections (1) communicipate the accorday. In a system typical tree accorday, in a system the tree of the various approximations which are supliced addressed to be rast of "Benefit's Method": (2) to examine the differences in numerical values of D, computed via cell-edge end cell-everaged normalizations and finally, to determine how large an uncentainty is incloduded into B, by the ambiguity in the datinition of call boundaries.

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(2) Equations (12) and (13') form another two-group set, but in this case $\Sigma_{s0}^{1\to 2} = -(1/2)$, $\Sigma_{s\ell}^{1\to 2} = 0$, $\ell > 0$. With h and h known, D_2 and \hat{D}_2 can be determined from Eqs. (36) and (36') respectively.

Coefficients D_2 and \hat{D}_2 , for diffusion parallel to the plates, have been computed in this way for a typical ZPPR cell configuration. The cell geometry is sketched in Fig. 1, and all relevant problem parameters appear in Table I. Cross sections in this table are spectrum weighted over the range from 1 to 10 MeV but it is felt that details of the origin of these cross sections are not important here. We are interested only in an estimate of the accuracy of Benoist's diffusion coefficient rather than the exact value of this coefficient in some particular lattice.

To compute D_y we have solved Eqs. (12) and (39) in various S_n approximations characterized, in Table II, as DP_3-P_7 , DP_4-P_9 , and DP_5-P_{11} . Here the designation DP_5-P_{11} refers to an S_n approximation with

- (1) 12 double-Gauss quadrature weights and ordinates, appropriate to a double- P_5 approximation; and
- (2) delta-function scattering from Group 1 into Group 2, represented in a P_{11} approximation.

The other designations have corresponding interpretations. In the computation of \hat{D}_2 , Eqs. (12) and (13') were again solved in DP₃, DP₄, and DP₅ approximations, but with anisotropic scattering from Group 1 into Group 2 suppressed, as indicated in the lower rows of Table II. It is very clear from Table II that Benoist's method, which yields \hat{D}_2 instead of D₂, is extremely accurate in this case despite the strong anisotropy of the angular flux.

B. Diffusion Normal to Plates

Making use of the knowledge that $I^{(0,1)}$ is proportional to Ω_y , it is possible, as we have seen, to compute this quantity by solving Eq. (39) on standard S_n codes. Similarly standard S_n codes can be used to solve Eq. (13') for \hat{h} which, then, gives us both $\hat{I}^{(0,1)}$ and $\hat{I}^{(1,0)}$. The computation of $I^{(1,0)}$ is slightly more difficult.

The quantity $I^{(1,0)}$ is determined by Eq. (14), which differs from the usual neutron transport equation in two respects. First, the coupling term, $\mu R^{(0,0)}$ cannot be developed in a Legendre polynomial expansion of the required form, i.e.,

$$_{\mu R}^{(0,0)} \neq \sum_{\ell=0}^{\infty} \left(\frac{2\ell+1}{2}\right) \Sigma_{s\ell} R_{\ell}^{(0,0)} P_{\ell}(\mu)$$

for any set of numbers $\Sigma_{s\ell}$. Secondly, one can show that

$$I^{(1,0)}(x,\mu) = -I^{(1,0)}(x,-\mu), \quad x = x_{\tau} \text{ or } x = x_{p}.$$
 (53)

Equation (53) defines a boundary condition ("antisymmetry condition") which is not available in standard S_n codes. On the other hand, it is not difficult to write a two-group S_n code which permits the imposition of "antisymmetric" boundary conditions and, in addition, includes the term ${}_{\mu}R^{(0,0)}$ as a source into the second group. Such a code has been written, and used to solve Eqs. (12) and (14).

Essentially three different approximations are involved in the process which takesus from D_1 to \hat{D}_1 . First, one neglects the second term in the numerator of Eq. (35): second, one replaces the source term $\mu R^{(0,0)}$ with the source term $\mu \varphi$: finally, the scattering term in Eq. (14) is deleted. Since the angular flux in the test problem

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The quantity $1^{(L_{\rm coll})}$ is determined by Eq. (14), which differs from the usual neutron transport equation in two respects. Frist, the coupling term, ${\rm uR}^{(0,0)}$ cannot be developed in a Legendre polynomial expansion of the required form, i.e.,

for any set of numbers to Secondly, one can show that

$$(23) \qquad \qquad \mathbf{x} = \mathbf{x} \quad \text{ro. } \mathbf{y} = \mathbf{x} \qquad , \quad (\mathbf{x}, \mathbf{x}) \cdot (0, \mathbf{t})_{1} = (\mathbf{x}, \mathbf{x}) \cdot (0, \mathbf{t})_{1}$$

Equation (5) defines a boundary condition ("antisymmetry condition") which is not available in standard in codes. On the other hand, it is not difficult to write a two-group in odde which permits the imposition of antisymmetric" boundary conditions and, in addition, includes the term of (0,00) as a source into the second group. Such a code has been written, and used to take Eqs. (12) and (14).

Essentially three different approximations are favolved in the process which takes us from 0, it by. First, one neglects the second tend in the numerator of Eq. (35): second, one replaces the source term was finally, the scattering term in Eq. (14) is deleted. Since the angular flux in the spat problem

configuration is highly anisotropic, it is interesting to ask how much error is introduced into the effective diffusion coefficient by the second step alone.

Suppose that, in Eq. (14), we replace $\mu R^{(0,0)}$ by $\mu \phi$ without making any other changes. Define a function $\overline{I}^{(1,0)}$ such that

$$\mu \frac{\partial \bar{I}^{(1,0)}}{\partial x} + \Sigma_{t} \bar{I}^{(1,0)} = \frac{\Sigma_{s}}{4\pi} \int d\hat{\Omega} \bar{I}^{(1,0)} - \mu_{\phi} . \qquad (14")$$

Let

$$\bar{j}_{1,11} = -\int \hat{\Omega} d\hat{\Omega} \bar{I}^{(1,0)}$$
,

and

$$\bar{D}_1 = \int_{x_L}^{x_R} \bar{J}_{1,11} dx / \int_{x_L}^{x_R} \phi dx$$
, (35")

while

$$\bar{\bar{D}}_{1} \equiv \int_{x_{L}}^{x_{R}} j_{1,11} dx / \int_{x_{L}}^{x_{R}} \phi dx$$
 (35"')

We see that the difference between \bar{D}_1 and $\bar{\bar{D}}_1$ reflects only the effect of anisotropy in $R^{(0,0)}$. 13

Values of $\bar{\mathbb{D}}_1$ and $\bar{\bar{\mathbb{D}}}_1$, computed in various S_n approximations, are listed in Table III. It will be seen that the anisotropy in the source term has no appreciable influence on the integral of the effective current $\mathbf{j}_{1,11}$. It seems remarkable that this should be true, in view of the fact that the flux, $R^{(0,0)}$, is so strongly anisotropic.

In Table IV we list values of D $_{x}$ computed according to various prescriptions. Diffusion coefficients which appear in the first row of numbers are computed from the Benoist definitions: $D_{1}^{A}(x_{B})$ and $D_{1}^{B}(x_{B})$ are "exact" Benoist diffusion coefficients, defined in Eq. (43), while \hat{D}_{1} is the "approximate" Benoist diffusion coefficient defined via Eq. (35'). It is this last diffusion coefficient which one would refer to, customarily, as the diffusion coefficient given by Benoist's method. We see that $D_{1}^{A}(x_{B})$ and $D_{1}^{B}(x_{B})$ differ by about 2%. On the other hand, since $\hat{D}_{2} \approx 2.88$ (see Table II), \hat{D}_{1} and \hat{D}_{2} differ by about 4%. Thus, the magnitude of the anisotropic effect is uncertain by 50%.

If, in Eq. (14) we simply replace the coupling term, $\mu R^{(0,0)}$, by the approximate coupling term $\mu \phi$, as in Eq. (14"), we get $\bar{I}^{(1,0)}$ in place of $I^{(1,0)}$. Suppose that we use the currents $\bar{J}_{1,11}(x_B)$ to define diffusion coefficients in place of the "exact" current $j_{1,11}(x_B)$. Diffusion coefficients so defined are listed in the second row of numbers in Table IV. As one might expect, the anisotropy of the flux has a much greater effect on the value of $j_{1,11}$ at individual points than it has on the volume integral of $j_{1,11}$. In fact the use of the scalar flux instead of the angular flux cuts in half the spread between the two permissible diffusion coefficients.

It turns out that the scalar flux, ϕ , varies much more over the test problem configuration, than does the effective current $j_{1,11}$. As a result the two cell-edge normalized diffusion coefficients, which appear in the last row of Table IV, are much farther apart than the corresponding coefficients as defined by Benoist. Moreover, they are much farther apart than the Benoist x and y diffusion coefficients, \hat{D}_1 and \hat{D}_2 . Thus, the spread between permissible values of the Bonalumi x diffusion coefficient totally obscures any anisotropic diffusion effect in the ZPPR lattice.

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problem configuration, then does the effective current 14.14. As a result the succession conficuency and the succession of the succession

V. CRITERIA FOR THE VALIDITY OF THE HOMOGENIZATION PROCESS

We see that there are substantial differences between the x diffusion coefficients as defined by Benoist and Bonalumi. Certainly we are left in an awkward position if we accept Bonalumi's definition, since the spread in permissible x diffusion coefficients is, then, so large. It does not follow, however, that Bonalumi's definition is wrong, or that Benoist's definition is right. In fact we have, at this point, adopted no criterion by which to judge either definition.

It is true that Selengut's equivalence principle 11 leads unambiguously to a definition of effective diffusion coefficients in certain circumstances. Selengut assumes, in Ref. 11, that diffusion theory is valid and that the absorption cross section vanishes. The direct application of Selengut's principle under more general conditions is not an entirely straightforward extension of his work and we prefer, here, to explore other approaches.

A. Assessment of the Performance of Homogenized Diffusion Coefficients

Consider, again, the one-energy transport equation, Eq. (1), and assume for simplicity that B $_y$ = 0. Given a lattice cell with boundaries at \mathbf{x}_{L} and \mathbf{x}_{R} , define

$$\bar{\Phi}_{\text{HET}} = \int_{\mathbf{x}_{L}}^{\mathbf{x}_{R}} \Phi_{\text{HET}}(\mathbf{x}) d\mathbf{x}/T$$
 (54)

Here $\Phi_{HET}(x)$ is the scalar flux in the heterogeneous assembly and T = $x_R - x_L$. It is clear that

$$\bar{\Phi}_{\text{HET}} = \bar{Q}/\left[\bar{\Sigma}_{\mathbf{a}} + D_1 B^2\right], \qquad (55)$$

$$\bar{Q} = \int_{x_L}^{x_R} q(x) \cos (Bx) dx/T, \qquad (56)$$

$$\overline{\Sigma}_{a} = \int_{x_{L}}^{x_{R}} \phi(x) \Sigma_{a}(x) dx / \int_{x_{L}}^{x_{R}} \phi(x) dx , \qquad (57)$$

$$D_{1} = \int_{x_{L}}^{x_{R}} (\partial/\partial x) J_{x} dx / \int_{x_{L}}^{x_{R}} \phi(x) dx .$$
 (58)

It will be seen, on comparison with Eq. (40), that D_1 is precisely the x diffusion coefficient as defined by Benoist, but it should be noted that \bar{Q} and $\bar{\Sigma}_a$ are functions of the buckling. To order B^2

$$\bar{Q} = Q^{(0)} + Q^{(2)}B^2$$
, $Q^{(0)} = \bar{q} \cos(Bx_0)$, $\bar{q} = \int_{x_L}^{x_R} q(x) dx/T$, (59)

$$\bar{\Sigma}_{a} = \Sigma_{a}^{(0)} + \Sigma_{a}^{(2)} B^{2}$$
, $\Sigma_{a}^{(0)} = \int_{x_{L}}^{x_{R}} \phi(x) \Sigma_{a}(x) dx / \int_{x_{L}}^{x_{R}} \phi(x) dx$. (60)

Thus we may write

$$\overline{\Phi}_{HET} = \frac{\left[Q^{(0)} + Q^{(2)}B^{2}\right]}{\left[\sum_{a}^{(0)} + \left(\sum_{a}^{(2)} + D_{1}\right)B^{2}\right]}.$$
(61)

In the homogenized assembly one generally takes, as the effective absorption cross section, the quantity

$$\left(\Sigma_{\mathbf{a}}\right)_{\mathbf{HOM}} = \int_{\mathbf{x}_{\mathbf{L}}}^{\mathbf{x}_{\mathbf{R}}} \phi(\mathbf{x}) \Sigma_{\mathbf{a}}(\mathbf{x}) d\mathbf{x} / \int_{\mathbf{x}_{\mathbf{L}}}^{\mathbf{x}_{\mathbf{R}}} \phi(\mathbf{x}) d\mathbf{x}$$

$$= \Sigma_{\mathbf{a}}^{(0)},$$
(62)

while the source density is given by the expression

$$Q_{HOM} = \bar{q} \cos (Bx) . \tag{63}$$

Expanding in powers of B and averaging over the cell we find that

$$\bar{Q}_{HOM} = Q^{(0)} - (1/24)B^2T^2\bar{q} \cos(Bx_0),$$

$$= Q^{(0)} - (1/24)T^2B^2Q^{(0)}.$$
(64)

Thus, given a homogenized x diffusion coefficient D_x ,

$$\overline{\Phi}_{HOM} = \frac{\overline{\mathbb{Q}^{(0)} - (1/24)T^2B^2\mathbb{Q}^{(0)}}}{\overline{\mathbb{D}_a^{(0)} + \mathbb{D}_xB^2}}.$$
(65)

If $\Delta \equiv Q^{(2)} - (1/24) T^2Q^{(0)}$, then

$$\overline{\Phi}_{HOM} = \frac{\left[Q^{(0)} + Q^{(2)}B^2 - B^2\Delta\right]}{\left[\Sigma_{\mathbf{a}}^{(0)} + D_{\mathbf{x}}B^2\right]},$$
(66)

so that, to order B2,

$$\overline{\Phi}_{HOM} = \frac{\left[Q^{(0)} + Q^{(2)}B^2\right]}{\sum_{a}^{(0)} + \left[D_{x} + \sum_{a}^{(0)} \left(\Delta/Q^{(0)}\right)\right]}.$$
(67)

From Eqs. (61) and (67) it is clear that $\bar{\Phi}_{\mbox{HOM}}$ and $\bar{\Phi}_{\mbox{HET}}$ will be different unless

$$D_{x} = D_{1} + \Sigma_{a}^{(2)} - \Sigma_{a}^{(0)} \left(\Delta/Q^{(0)} \right) . \tag{68}$$

We see that if the effective absorption cross section and the source are defined as in Eqs. (62) and (63) respectively, then both the Bonalumi and Benoist prescriptions will yield incorrect average fluxes within the

boundaries of each cell. Further, even if we were to use Eq. (68) to define an effective diffusion coefficient (again double-valued), the absorption rate, AR, in the cell would be given, to order B^2 , by the expression

$$AR = \left(\Sigma_a^{(0)} + \Sigma_a^{(2)} B^2\right) \overline{\Phi}_{HOM} T , \qquad (69)$$

and

AR
$$\neq \Sigma_{a}^{(0)} \overline{\Phi}_{HOM}^{T}$$
.

We do not mean to suggest, at this point, that a prescription involving a buckling-dependent absorption cross section would actually be practical. Rather it is our intention to point out that the defects in present homogenization schemes will not be easy to remedy.

When $B_x=0$, $B_y\ne0$, we again find, by similar arguments, that the Benoist method gives an incorrect average flux in the interval which corresponds to the extent of any cell. In this case, however, it turns out, when one uses Benoist's D_2 as the diffusion coefficient, that $\Sigma_a^{(0)} \bar{\Phi}_{HOM}(\underline{r}_0)$ is the correct average absorption rate in the cell centered at \underline{r}_0 . Again we recall that the Benoist and Bonalumi D_v are the same.

It seems important to be aware of these deficiencies in the Bonalumi and Benoist methods, deficiencies which we have noted in the Bonalumi and Benoist treatments of the inhomogeneous transport equation. But it is not necessarily true that one should go so far as to redefine diffusion coefficients with the inhogeneous transport equation specifically in mind. In fact it may be better, at this point, to turn our attention from inhomogeneous to eigenvalue problems.

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B. Reformulation of Definition of Effective Diffusion Coefficients

In our notation the one-group transport equation with fission and isotropic scattering takes the form

$$\mu(\partial R/\partial x) + \Sigma_{\mathbf{t}} R = \left(\Sigma_{\mathbf{s}}/4\pi\right) \phi + (1/\lambda) \left(\nu \Sigma_{\mathbf{f}}/4\pi\right) \phi + (\widehat{\Omega} \cdot \underline{B}) I, \qquad (70)$$

$$\mu(\partial I/\partial x) + \Sigma_{t} I = \left(\Sigma_{s}/4\pi\right)\psi + (1/\lambda)\left(\nu\Sigma_{f}/4\pi\right)\psi - \left(\hat{\Omega} \cdot \underline{B}\right)R, \qquad (71)$$

where

$$\phi \equiv \int R d\hat{\Omega}$$
 (72)

and

$$\psi \equiv \int I \ d\hat{\Omega} \ . \tag{73}$$

Suppose we consider the term $(\hat{\Omega} \cdot \underline{B})I$ in Eq. (70) as a perturbation, defining "unperturbed" eigenvalue equations as follows:

$$\mu(\partial \tilde{R}/\partial x) + \Sigma_{t}\tilde{R} = \left(\Sigma_{s}/4\pi\right)\tilde{\phi} + (1/\lambda_{0})\left(\nabla\Sigma_{t}/4\pi\right)\tilde{\phi}, \qquad (74)$$

$$\mu(\partial \tilde{\mathbf{I}}/\partial \mathbf{x}) + \Sigma_{\mathbf{t}} \tilde{\mathbf{I}} = \left(\Sigma_{\mathbf{s}}/4\pi\right)\tilde{\psi} + (1/\lambda_0)\left(\nabla\Sigma_{\mathbf{f}}/4\pi\right)\tilde{\psi} - (\tilde{\Omega} \cdot \underline{B})\tilde{R} . \tag{75}$$

It will be seen that each unperturbed eigenvalue, λ_0 , is actually degenerate with eigenvectors

$$\underline{\mathbf{v}}_1 = \begin{pmatrix} \tilde{\mathbf{R}} \\ \tilde{\mathbf{I}} \end{pmatrix}, \qquad \underline{\mathbf{v}}_2 = \begin{pmatrix} 0 \\ \tilde{\mathbf{R}} \end{pmatrix}.$$
 (76)

The unperturbed adjoint equations appear below:

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$$-\mu(\partial \tilde{R}^{\star}/\partial x) + \Sigma_{t}\tilde{R}^{\star} = \left(\Sigma_{s}/4\pi\right)\tilde{\phi}^{\star} + (1/\lambda_{0})\left(\nu\Sigma_{f}/4\pi\right)\tilde{\phi}^{\star} - (\tilde{\Omega} \cdot \underline{B})\tilde{I}^{\star}, (77)$$

$$-\mu(\partial \tilde{\mathbf{I}}^{\star}/\partial \mathbf{x}) + \Sigma_{\mathbf{t}}\tilde{\mathbf{I}}^{\star} = \left(\Sigma_{\mathbf{s}}/4\pi\right)\tilde{\psi}^{\star} + (1/\lambda_{0})\left(\nabla\Sigma_{\mathbf{f}}/4\pi\right)\tilde{\psi}^{\star}, \qquad (78)$$

Again, for each λ_0 there are two eigenvectors which we may write as follows:

$$\underline{V}_{1}^{\star} = \begin{pmatrix} \widetilde{R}(-\mu) \\ 0 \end{pmatrix}, \qquad \underline{V}_{2}^{\star} = \begin{pmatrix} -\widetilde{I}(-\widehat{\Omega}) \\ \widetilde{R}(-\mu) \end{pmatrix}. \tag{79}$$

Let

$$\Delta H = \begin{pmatrix} 0 & -(\hat{\Omega} \cdot \underline{B}) \\ 0 & 0 \end{pmatrix}.$$

It is easy to see that

$$\left\langle \underbrace{v \dagger v}_{j} \right\rangle = 0 , \quad i \neq j ,$$
 (80)

$$\left\langle \underline{V}_{\mathbf{j}}^{\star}(\Delta H)\underline{V}_{\mathbf{j}}\right\rangle = 0$$
 , $i \neq j$. (81)

Here

$$\langle UV \rangle = \int d\hat{\Omega} \int_{\mathbf{x}_L}^{\mathbf{x}_R} U(\mathbf{x}, \hat{\Omega}) V(\mathbf{x}, \hat{\Omega}) d\mathbf{x}$$

Further one can show that

$$\begin{split} &\left\langle \underline{V}_{1}^{\star}(\Delta H)\underline{V}_{1}\right\rangle = \left\langle \underline{V}_{2}^{\star}(\Delta H)\underline{V}_{2}\right\rangle \text{,} \\ &\left\langle \underline{V}_{1}^{\star}\left(\nu \Sigma_{\mathbf{f}}\mathbf{I}\right)\underline{V}_{1}\right\rangle = \left\langle \underline{V}_{2}^{\star}(\nu \Sigma_{\mathbf{f}}\mathbf{I})\underline{V}_{2}\right\rangle \text{,} \end{split}$$

where I is the identity operator. Therefore it follows from degenerate perturbation theory that there is only one perturbed eigenvalue, given by the expression

$$(1/\lambda) = (1/\lambda_0) + \left\langle \underline{V}_1^{\star}(\Delta H)\underline{V}_1 \right\rangle / \left\langle \underline{V}_1^{\star}(\nu \Sigma_f I)\underline{V}_1 \right\rangle . \tag{82}$$

More explicitly

$$(1/\lambda) = (1/\lambda_0) - \int d\Omega \int_{\mathbf{x}_{\underline{\mathbf{I}}}}^{\mathbf{x}_{\underline{\mathbf{R}}}} \tilde{\mathbf{R}}(-\mu)(\hat{\Omega} \cdot \underline{\mathbf{B}})\tilde{\mathbf{I}}(\hat{\Omega}) dx/F. \qquad (83)$$

Here

$$F \equiv \int_{\mathbf{x}_{L}}^{\mathbf{x}_{R}} \left(v \Sigma_{\mathbf{f}} \right) \tilde{\phi}^{2} dx .$$

Define \tilde{I}_x and \tilde{I}_y such that

$$\mu(\partial \tilde{I}_{x}/\partial x) + \Sigma_{t}\tilde{I}_{x} = (\Sigma_{s}/4\pi)\tilde{\psi} + (1/\lambda_{0})(\nabla \Sigma_{f}/4\pi)\tilde{\psi} - \mu B_{x}\tilde{R}, \qquad (84)$$

$$\mu(\tilde{I}_{y}/\partial y) + \Sigma_{t}\tilde{I}_{y} = -\Omega_{y}B_{y}\tilde{R}, \qquad (85)$$

$$\tilde{\psi} = \int d\hat{\Omega} \tilde{I}_{x}.$$

It can easily be shown that Eqs. (84) and (85) \underline{do} have solutions, despite the fact that $(1/\lambda_0)$ is an eigenvalue of the corresponding homogeneous equations. Further $\tilde{I}=\tilde{I}_x+\tilde{I}_y$ and, finally,

$$-\int d\hat{\Omega} \int_{\mathbf{x_L}}^{\mathbf{x_R}} \tilde{R}(-\mu)(\hat{\Omega} \cdot \underline{B})\tilde{I}(\hat{\Omega}) dx = B_{\mathbf{x_T}}^2 + B_{\mathbf{y_T}}^2, \qquad (86)$$

where

$$\begin{split} \tau_{_{\mathbf{X}}} &\equiv & -\int \, d\hat{\Omega} \int_{\mathbf{x}_{_{\mathbf{L}}}}^{\mathbf{x}_{_{\mathbf{R}}}} \, \mu R(-\mu) \, \tilde{I}_{_{\mathbf{X}}}(\mu) \, \, \mathrm{d}x/F \;\;, \\ \tau_{_{\mathbf{y}}} &\equiv & -\int \, d\hat{\Omega} \, \int_{\mathbf{x}_{_{\mathbf{R}}}}^{\mathbf{x}_{_{\mathbf{R}}}} \, \Omega_{_{\mathbf{y}}} \tilde{R}(-\mu) \, \tilde{I}_{_{\mathbf{y}}}(\hat{\Omega}) \, \, \mathrm{d}x/F \;\;. \end{split}$$

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From Eqs. (83) amd (86) it follows that

$$(1/\lambda) = (1/\lambda_0) + B_{\mathbf{x}}^2 + B_{\mathbf{y}}^2 . \tag{87}$$

Now

$$\lambda_0 = \sqrt{\Sigma_f^{(0)}} / \overline{\Sigma_a^{(0)}}, \qquad (88)$$

where

$$\overline{\nu}_{\mathbf{f}}^{(0)} = \int_{\mathbf{x}_{\mathbf{L}}}^{\mathbf{x}_{\mathbf{R}}} \left(\nu \Sigma_{\mathbf{f}} \right) \tilde{\phi}(\mathbf{x}) \, d\mathbf{x} / \int_{\mathbf{x}_{\mathbf{L}}}^{\mathbf{x}_{\mathbf{R}}} \tilde{\phi}(\mathbf{x}) \, d\mathbf{x} , \qquad (89)$$

$$\overline{\Sigma}^{(0)} = \int_{\mathbf{x}_{L}}^{\mathbf{x}_{R}} \Sigma_{\mathbf{a}}^{\tilde{\phi}}(\mathbf{x}) d\mathbf{x} / \int_{\mathbf{x}_{L}}^{\mathbf{x}_{R}} \tilde{\phi}(\mathbf{x}) d\mathbf{x} . \tag{90}$$

Therefore we may write Eq. (87) in the form

$$(1/\lambda) = \left[\overline{\Sigma}_{\mathbf{a}}^{(0)} / \overline{\nu}_{\mathbf{f}}^{(0)} \right] \left\{ 1 + \left[\overline{\nu}_{\mathbf{f}}^{\Sigma}_{\mathbf{f}}^{(0)} / \overline{\Sigma}_{\mathbf{a}}^{(0)} \right] \left(\tau_{\mathbf{x}} B_{\mathbf{x}}^{2} + \tau_{\mathbf{y}} B_{\mathbf{y}}^{2} \right) \right\},$$

$$= \left\{ \overline{\Sigma}_{\mathbf{a}}^{(0)} + \left[\overline{\nu}_{\mathbf{f}}^{\Sigma}_{\mathbf{f}}^{(0)} \right] \tau_{\mathbf{x}} B_{\mathbf{x}}^{2} + \left[\overline{\nu}_{\mathbf{f}}^{\Sigma}_{\mathbf{f}}^{(0)} \right] \tau_{\mathbf{y}} B_{\mathbf{y}}^{2} \right\} / \overline{\nu}_{\mathbf{f}}^{\Sigma}_{\mathbf{f}}^{(0)}. \tag{91}$$

It will be seen from Eq. (91) that, if we take $\overline{\Sigma}^{(0)}$ and $\overline{\nabla\Sigma}_{\mathbf{f}}^{(0)}$ as the "equivalent homogenized" $\Sigma_{\mathbf{a}}$ and $\nabla\Sigma_{\mathbf{f}}$, respectively, then $\left[\overline{\nabla\Sigma}_{\mathbf{f}}^{(0)}\right]^{\mathsf{T}}_{\mathbf{x}}$ plays the role of $D_{\mathbf{y}}$, while $\left[\overline{\nabla\Sigma}_{\mathbf{f}}^{(0)}\right]^{\mathsf{T}}_{\mathbf{y}}$ plays the role of $D_{\mathbf{y}}$. We are led, then, to define

$$D_{\mathbf{x}}^{(\lambda)} = \left[-\int d\hat{\Omega} \int_{\mathbf{x}_{L}}^{\mathbf{x}_{R}} \mu \tilde{R}(-\mu) \tilde{I}_{\mathbf{x}}(\mu) d\mathbf{x} \right] \int_{\mathbf{x}_{L}}^{\mathbf{x}_{R}} \left(\nu \Sigma_{\mathbf{f}} \right) \tilde{\phi}(\mathbf{x}) d\mathbf{x} / \int_{\mathbf{x}_{L}}^{\mathbf{x}_{R}} \left(\nu \Sigma_{\mathbf{f}} \right) \phi^{2}(\mathbf{x}) d\mathbf{x} , \quad (92)$$

$$D_{\mathbf{y}}^{(\lambda)} = \left[-\int d\hat{\Omega} \int_{\mathbf{x}_{L}}^{\mathbf{x}_{R}} \Omega_{\mathbf{y}} R(-\mu) \tilde{\mathbf{I}}_{\mathbf{y}}(\hat{\Omega}) d\mathbf{x} \right] \int_{\mathbf{x}_{L}}^{\mathbf{x}_{R}} \left(v \Sigma_{\mathbf{f}} \right) \tilde{\phi}(\mathbf{x}) d\mathbf{x} / \int_{\mathbf{x}_{L}}^{\mathbf{x}_{R}} \left(v \Sigma_{\mathbf{f}} \right) \tilde{\phi}^{2}(\mathbf{x}) d\mathbf{x} . (93)$$

Suppose that, in Eq. (82), we approximate the importance function, $\underline{v}_{1}^{\star}$, by its average over space and solid angle. We find, in this approxima-

$$D_{x}^{(\lambda)} \approx \int_{x_{L}}^{x_{R}} \tilde{j}_{1,11} dx / \int_{x_{L}}^{x_{R}} \tilde{\phi}(x) dx , \qquad (94)$$

and,

$$D_{y}^{(\lambda)} \approx \int_{x_{L}}^{x_{R}} \tilde{j}_{1,22} dx / \int_{x_{L}}^{x_{R}} \tilde{\phi}(x) dx . \qquad (95)$$

Further, if we now compute $\tilde{j}_{1,11}$ and $\tilde{j}_{1,22}$ by Benoist's collision probability methods, $D_x^{(\lambda)}$ and $D_y^{(\lambda)}$ become, identically, Benoist's \hat{D}_1 and \hat{D}_2 . Thus there is a close connection between Benoist's diffusion coefficients and the diffusion coefficients required to preserve the eigenvalue during homogenization. Perhaps this close connection gives us a justification of some sort for the use of Benoist's method: at the moment we see no similar justification for the use of Bonalumi's method.

We digress here to note that the effective diffusion coefficients defined in Eqs. (92) and (94) differ from those derived earlier by Williams. Williams on comparing Eq. (77) in Ref. 14 with our Eq. (40), one finds that Williams'x diffusion coefficient, \bar{D}_x , is identical with the Benoist D_1 . Williams apparently concludes that the diffusion coefficient \bar{D}_x (or D_1), used in conjunction with $\bar{\Sigma}_a^{(0)}$ and $\bar{\nu}_f^{(0)}$, reproduces the heterogeneous lattice eigenvalue. Yet it would seem that this cannot be true, simply because D_1 is double-valued if for no other reason.

It is difficult to compare Williams' work, in detail, with our own since the mathematical techniques used here and in Ref. 14 are, formally, quite different. We believe, however, that the discrepancies between our results and those reported by Williams can be traced back to a fundamental assumption embodied in Eq. (3) of Ref. 14. Williams postulates that $k_{\rm eff} = k_{\infty} P$, where P is the nonleakage probability. We have argued, above,

that $k_{\rm eff}$ and k_{∞} differ, not only because of the direct effect of leakage, but also because (to order B^2) the leakage modifies the effective absorption and fission cross sections. We see no treatment of such indirect effects in Williams' derivation.

Diffusion coefficients defined by Eqs. (92) and (93) have not yet been computed for our ZPPR test problem configuration. It is possible, however, to make a rough estimate of the ratios between these coefficients, on the one hand, and Benoist's on the other. We have already seen that approximations based on the assumption that R is isotropic tend to be very accurate. It has also been noted earlier that $\mathbf{j}_{1,11}$ is nearly constant over the ZPPR cell and, in fact, we observe that $\mathbf{j}_{1,22}$ is also nearly constant. If it is assumed that R is isotropic, and that both $\mathbf{j}_{1,11}$ and $\mathbf{j}_{1,22}$ are constant, we find that

$$\begin{bmatrix} D_{\mathbf{x}}^{(\lambda)}/\hat{D}_{1} \end{bmatrix} \approx \begin{bmatrix} \int_{\mathbf{x}_{L}}^{\mathbf{x}_{R}} \left(v \Sigma_{\mathbf{f}} \right) \tilde{\phi} d\mathbf{x} / \int_{\mathbf{x}_{L}}^{\mathbf{x}_{R}} \left(v \Sigma_{\mathbf{f}} \right) \tilde{\phi}^{2} d\mathbf{x} \end{bmatrix} \begin{bmatrix} \mathbf{x}_{R} & \tilde{\phi} d\mathbf{x} / T \end{bmatrix}$$

$$\approx \begin{bmatrix} D_{\mathbf{y}}^{(\lambda)}/\hat{D}_{2} \end{bmatrix}. \tag{96}$$

In order to make an estimate of the value of the integrals on the right-hand side of Eq. (96), we assume, further, that ϕ is approximately equal to the scalar flux, ϕ , computed earlier, in our fixed-source test problem. It will be recalled that, in this fixed source problem, the source in each region was taken to be equal to $\nu \Sigma_f$ in that region. It seems not unreasonable, therefore, to assume that ϕ and ϕ have roughly the same shape. At any rate if we make this assumption we come to the conclusion that

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$$\begin{bmatrix} D_{\mathbf{x}}^{(\lambda)}/\hat{D}_1 \end{bmatrix} \stackrel{\sim}{\sim} \begin{bmatrix} D_{\mathbf{y}}^{(\lambda)}/\hat{D}_2 \end{bmatrix} \stackrel{\sim}{\sim} 0.964 , \qquad (97)$$

i.e. that Benoist's D's are too small, in this case, by about three to four percent.

We believe that Eqs. (92) and (93) can be generalized straightforwardly to the multigroup case, at least in situations where the group-togroup scattering is taken to be isotropic. Generalized versions of these equations could be used to test Benoist's method, or to correct Benoist's diffusion coefficients when corrections are deemed necessary. It should be stressed, at this point, that the proposed new definitions of D and D are contrived for one purpose alone: they are designed to reproduce, in the homogenized lattice, the eigenvalue of the heterogeneous lattice. The eigenvalue in the homogenized lattice will be correct to order B2 if the new diffusion coefficients are used in conjunction with the bucklingindependent one-group parameters defined in Eqs. (89) and (90). On the other hand, edited reaction rates (for any given power level) will not be correct to order B2 unless the reaction cross sections are buckling dependent; and, unfortunately it is not clear that the use of bucklingdependent reaction cross sections would actually be feasible in the analysis of real reactors. Thus the new prescription for the computation of diffusion coefficients shares some of the weaknesses of older prescriptions.

How important these weaknesses are, from a practical point of view, we cannot say. Further it should be pointed out that very little is known, at this time, about the performance of any homogenization scheme near interfaces. In view of the difficulty of a more thorough theoretical analysis

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it seems clear that, ultimately, only detailed Monte Carlo calculations can give us the information we need for definitive tests of our and other homogenization procedures.

VII. CONCLUSIONS

In the particular version of the ZPPR which we have studied here the probability of leakage out of the core is, approximately, 30%, and the leakage probabilities in the x, y, and z directions are roughly equal. Further the Benoist x diffusion coefficient, D1, turns out to be almost equal to the diffusion coefficient, D, computed from the flux-weighted transport cross section. On the other hand, the y and z Benoist diffusion coefficients, D_2 and D_3 , are greater than \bar{D} by about 4%. It follows that when we use the Benoist method, taking D_1 , D_2 , and D_3 (in place of \bar{D}) for the x, y, and z diffusion coefficients, we lower the eigenvalue, k_{eff} , by about 0.8%. If, now, we assume that D_1 is uncertain by 2%, an amount corresponding to the spread between the two permissible values of D_1 , we conclude that k_{off} is uncertain by roughly 0.2%. Such an uncertainty is not particularly significant, and is fairly small compared to the 0.8% change in k caused, in toto (according to Benoist's method), by anisotropic diffusion. In contrast the 11% spread in Bonalumi's x diffusion coefficient gives rise to a 1% uncertainty in eigenvalue, an uncertainty which is significant, and is no smaller than the whole anisotropy effect. Moreover Bonalumi's definition of effective diffusion coefficients seems as appealing, intuitively, as Benoist's.

Since intuition does not seem to lead us to one unique definition of \mathbf{D}_1 , we have found it necessary to formulate a precise objective of some

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sort for the homogenization process. The objective we have chosen is quite simple. We wish to construct buckling independent group parameters such that the homogeneous eigenvalue (i.e. the eigenvalue in the homogenized lattice) will be equal to the heterogeneous eigenvalue to order B^2 . Suitable parameters are defined, for one-group problems, in Section V. It seems clear that corresponding multigroup parameters can be obtained by straightforward generalization of the methods of Section V if the P_1 transfer matrix is diagonal.

The diffusion coefficients defined in Section V are ratios of integrals whose integrands contain importance functions. If we approximate these importance functions by their average values we find that our $D_{\mathbf{x}}^{(\lambda)}$ and $D_{\mathbf{y}}^{(\lambda)}$ become identically the same as Benoist's \hat{D}_1 and \hat{D}_2 , respectively. This close connection between \hat{D} and the diffusion coefficients required to preserve \mathbf{k}_{eff} seems to provide some measure of justification for the use of Benoist's method.

It is interesting to note, however, that if one advocates the use of Benoist's method on such grounds one cannot, any longer, consider the term

$$\Delta D_1 = \int_{\mathbf{x}_L}^{\mathbf{x}_R} (\mathbf{x} - \mathbf{x}_0) (\partial \mathbf{j}_{1,11} / \partial \mathbf{x}) d\mathbf{x} / \int_{\mathbf{x}_L}^{\mathbf{x}_R} \phi d\mathbf{x}$$

as a correction to \hat{D}_1 . The quantity \hat{D}_1 will generally lie somewhere within the interval bounded by the two values of D_1 . By adding ΔD_1 to \hat{D}_1 one moves the x diffusion coefficient, from some point inside this interval, to a new point close to one of its boundaries. But it is difficult to see why either boundary value, $D_1\{x_B\}$, should be any more correct than \hat{D}_1 .

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If we take $D_{\mathbf{x}}^{(\lambda)}$ and $D_{\mathbf{y}}^{(\lambda)}$ to be the "true" homogenized diffusion coefficients there does not seem to be any simple expression for the errors in \hat{D}_1 and \hat{D}_2 . In Section V we have tried to estimate the magnitude of these errors in our test problem and have concluded that \hat{D}_1 and \hat{D}_2 are too large by about 3.4%. Such errors in Benoist's D's would produce a 1% error in k_{eff} in the reactor configuration under consideration here. Now, our test problem is a one-group problem with group parameters covering the range from 1 to 10 MeV. In a multigroup adjoint computation the group in question would contain "slowing-down" sources coupling it to groups of lower energies. Because of the absence of such fictitious slowing-down sources in the one-group adjoint equations it is possible that the one-group and multigroup importance functions will be guite different in shape. Therefore one cannot assume that our estimate of the errors in Benoist's D's will be very accurate. Nevertheless our results do seem to indicate that these errors may be significant and should be examined further.

Many weaknesses in the treatment of anisotropic diffusion remain. The group parameters which enter into eigenvalue calculations would, according to our proposal, be buckling independent. But if we are to compute reaction rates which are correct to order B² the cross sections used to compute these reaction rates cannot be buckling independent. We see no way to circumvent this difficulty. Further the quantities $D_{\mathbf{x}}^{(\lambda)} B_{\mathbf{x}}^2 \Phi \text{ and } D_{\mathbf{y}}^{(\lambda)} B_{\mathbf{y}}^2 \Phi \text{ are not simply leakage rates since } D^{(\lambda)} \text{ contains, implicitly, contributions due to the buckling dependence of } \nabla \Sigma_{\mathbf{f}} \text{ and } \Sigma_{\mathbf{a}}.$ It is possible that the use of such a diffusion coefficient is not appropriate near interfaces. On the other hand, there seems to be no good

theoretical foundation for any homogenization prescription near interfaces. Clearly, then, we cannot claim to have solved all the problems involved in the computation of homogenized group constants. Yet, despite all the remaining difficulties, it still seems important to require that a homogenization procedure should preserve the heterogeneous eigenvalue, in an infinite lattice, to order B².

In closing we note that much of what has been said here is obviously relevant in other geometries, as well as in slab geometry. Clearly our arguments about eigenvalues and reaction rates are equally valid in any periodic lattice. Perhaps it is not quite so obvious that the Benoist and Bonalumi diffusion coefficients are generally double-valued in square and hexagonal cells, just as they are in slab cells. Yet this is true. Consider, for example, an array of rods in a square or hexagonal lattice. It is customary (and convenient) to define a unit cell with the rod at its center: but it is also possible to define a cell with a rod at each corner of its boundary. Corresponding to each of these two possible definitions of the unit cell we would get two values of the exact Benoist diffusion coefficient, and two values of the Bonalumi coefficients.

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In closing we note that much of what has been been to the country oun recipract in other geometries, as well as in slangeometry. Oleanly, oun arguments about elgenvalues and materium rates are equality value to any and Bonaium! Sermans at its not units so cerious, that the Bengue and Reasonal tells, just as they are in slab cells. Yet this is true, and hexagonal tells, just as they are in slab cells. Yet this is true. It is customary (and convenient) of genne a unit of i, with the cod at the countries of the example, an arror of genne a unit of i, with the cod at define of the customary. Corresponding to each of their the cod at definitions of the unit cell, we would ent ten values of the exact fencial definitions of the unit cell, we would ent ten values of the exact fencial

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- $^{7}\text{The reader may observe that } \pmb{\int} d\hat{\Omega} \ I^{\,(0\,\cdot\,1)}$ vanishes and we make use of this fact later.
 - 8 The definition of $x_{_{T}}$ and $x_{_{R}}$ will be discussed further in Section III.
 - 9See, for example, Ref. 3, Eq. (A-15).
- $^{10}\text{Since j}_{1,11}$ and ϕ are periodic we may take, as the value of \mathbf{x}_{B} , either \mathbf{x}_{L} or \mathbf{x}_{R} .
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TABLE I
Test Problem Parameters

(Left- and right-hand boundaries are symmetry planes. Source density has been set equal to $\nu \Sigma_{\bf f}$ in each region.)

	Region I (Uranium Oxide)	Region II (Sodium)	Region III (Uranium-Plutonium)
Thickness (cm)	1.0	1.25	0.25
Source Density	0.00998	0.	0.185
Σt	0.181551	0.0452915	0.252648
Σ _s 0	0.117890	0.0267661	0.0860426

E Problem Parameters

(Left. and mightwheel Washelms are symmetry planes source desirity has been set equal to use in each region.)

TABLE II

Parallel Diffusion Coefficients
in a Typical ZPPR Lattice

	DP ₃ -P ₇	DP4-P9	DP ₅ -P ₁₁
D ₂ (cm)	2.8705	2.8740	2.8768
	DP ₃ -P ₀	DP ₄ -P ₀	DP ₅ -P ₀
D ₂ (cm)	2.8613	2.8707	2.8798

 D_2 is computed from Eqs. (12), (36), and (39).

 \hat{D}_2 is the Benoist approximate D_2 , computed from Eqs. (12), (13'), and (36').

TABLE II

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D. 1s computed from Eqs. (12), (36), and (18)

U. is the Benoist approximate U., computed from Eqs. (127, (137), and (367).

TABLE III
Diffusion Coefficients Normal to Plates

	DP ₃ -P ₇	DP4-P9	DP ₅ -P ₁₁
Ō₁	2.759	2.765	2.769
	DP 3-P0	DP ₄ -P ₀	DP ₅ -P ₀
D ₁	2.772	2.771	2.771

 $\bar{\bar{D}}_1$ is computed from Eqs. (14) and (35"'): anisotropic source term $\mu R^{(0,0)}$.

 $\boldsymbol{\tilde{D}}_1$ is computed from Eqs. (14") and (35"): isotropic source term $\mu\phi$

Diffusion Coefficients Normal to Plant

Digits computed from Eqs. (14) and (35"): arreacropic source term on (0.02)

En is computed from Eqs. (14") and (35") isotropic source corm up.

TABLE IV

Coefficients for Diffusion Normal to Plates, According to Benoist's and Bonalumi's Prescriptions

D ₁ from Be	noist's Definiti	ons
$D_1^A(x_B)$	$D_1^B(x_B)$	D ₁
DP ₅	DP ₅	DP ₅
2.7775	2.7211	2.7677
$D_1^A(x_B)$	$D_1^B(x_B)$	
DP ₅	DP ₅	
source = μφ	source = μφ	
2.7754	2.7460	
D ₁ from Bo	nalumi's Definit	ion
$D_1^A(x_B)$	$D_1^B(x_B)$	
DP ₅	DP ₅	
2.9182	2.4378	

Conff quency for Distusion Normal re Flates, According to Bendar's and Ronalumits Presentanters

2.740	

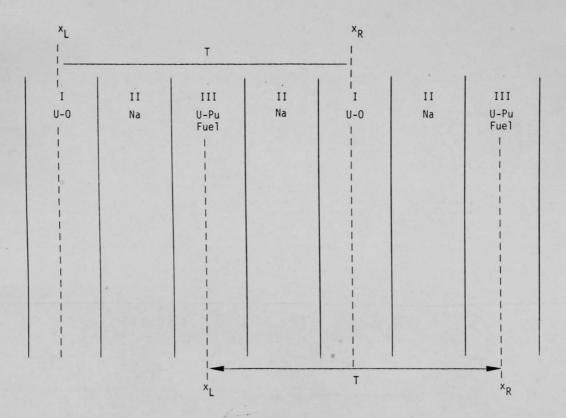
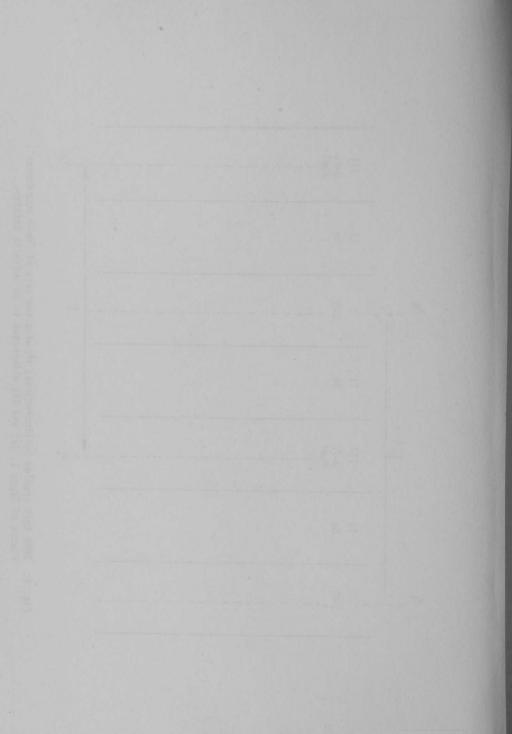


Fig. 1. ZPPR test problem configurations, showing two sets of "cell boundaries". Plates of Types I, II, and III alternates in an infinite lattice.



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